THE SCHRÖDINGER WAVE EQUATION FROM THE POINT OF VIEW OF SINGULAR INTEGRAL EQUATIONS

BY

DAVID WRIGHT STARR

A.B., Southern Methodist University. 1933

A.M., University of Illinois, 1937

AN ABSTRACT OF A THESIS

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN MATHEMATICS IN THE GRADUATE SCHOOL OF THE UNIVERSITY OF ILLINOIS, 1940

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I. INTRODUCTION

In an article, "Sur la théorie mathématique de l'équation de Schrödinger" in Arkiv För Matematik, Astronomi Och Fysik, Band 24B, 1933-34, Torsten Carleman has announced some results in regard to the Schrödinger Wave equation of quantum mechanics. This equation is a linear partial differential equation of elliptic type. It presents problems distinct from the classical type for elliptic partial differential equations.

These results are announced - without proof or with method of proof in part suggested. It is of interest to give in detail the proofs of some of the more important results.

The method in investigations of this type consists in applying the theory of singular integral equations due to Carleman.*

It appears that the importance of this method of approach, in the field under consideration, has been largely overlooked.

II. TRANSFORMATION TO AN INTEGRAL EQUATION

We consider an equation in partial derivatives in the Euclidean space of three dimensions of the form

$$(1) \qquad L(u) + \lambda u = f$$

where $L(u) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + c(x,y,z)\,u$ (c - a real function)

We generalize the notion of the Laplacian Δu. We consider a sphere K_ρ with center p and radius ρ in a domain D. We also consider an inner sphere S_ρ with center p and radius r. q is any point on the surface of the sphere.

Let us put

$$(2) \qquad A(p,q) = \frac{1}{r_{p,q}} + \frac{r_{p,q}}{\rho^2} - \frac{2}{\rho}$$

where $r_{p,q}$ is the distance between the points p and q.

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* Carleman, T.: Sur les Équations Intégrales Singulières a Novau Réel et Symétrique, Uppsala, 1923.
(in sequel referred to as (C))

We apply Green's formula to $u(q)$ and $A(p,q)$. We have

$$\iiint_{K_\rho - S_\eta} \left[u(q)\,\Delta A(p,q) - A(p,q)\,\Delta u(q)\right] d\omega_q =$$

$$(3)\quad = -\left\{\left(\iint_{K_\rho} - \iint_{S_\eta}\right)\left[A(p,q)\frac{\partial u(q)}{\partial n} - u(q)\frac{\partial A(p,q)}{\partial n}\right] d\sigma_q\right\}$$

(σ_q is element of surface

Now $r_{p,q} = \rho$ for q on the surface of K_ρ. So (2) or $A(p,q)$ becomes zero on the surface K_ρ and likewise for $\frac{\partial A(p,q)}{\partial n}$ since $\frac{\partial A(p,q)}{\partial n} = -\frac{1}{r^2} + \frac{1}{\rho^2}$

(3) becomes then for the right member

$$(3a)\quad \iint_{S_\eta}\left[A(p,q)\frac{\partial u(q)}{\partial n} - u(q)\frac{\partial A(p,q)}{\partial n}\right] d\sigma_q = G(p,\eta)$$

We show then that $\lim_{\eta \to 0} G(p,\eta) = 4\pi u(p)$. The value for $\Delta A(p,q)$ is found and these values for $G(p,\eta)$ and $\Delta A(p,q)$ are substituted with $\Delta u = \varphi(q)$ in (3) and we obtain an integral equation

$$(4)\quad u(p) - \frac{1}{2\pi\rho^2}\int_{K_\rho}\frac{1}{r_{p,q}}\,u(q)\,d\omega_q + \frac{1}{4\pi}\int_{K_\rho} A(p,q)\,\varphi(q)\,d\omega_q = 0$$

and we are led to the conclusion that if $\Delta u = \varphi(q) \subset L_2$ and if u is a solution of (1) with continuous first partials then u satisfies the integral equation. The equation determines $\varphi(q)$ in a unique manner and this coincides with the ordinary definition of Δu.

The Green formulas

$$(5)\quad \int_D \left(u\,L(v) - v\,L(u)\right) d\omega + \int_S \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right) d\sigma = 0$$

$$(6)\quad \int_D u\,L(v)\,d\omega + \int_D \left(\frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} + \frac{\partial u}{\partial z}\frac{\partial v}{\partial z} - cuv\right) d\omega + \int_S u\frac{\partial v}{\partial n}\,d\sigma = 0$$

are valid for the symbol Δu generalized under certain conditions.

Suppose $u(q)$ with continuous first partials satisfies (1) then u satisfies (4) with $\varphi(q) = f - (c+\lambda)u \subset L_2$ (if $f, c \subset L_2$). Using (4) we have

$$(7)\quad u(p) = \frac{1}{2\pi\rho^2}\int_{K_\rho}\frac{1}{r_{p,q}}\,u(q)\,d\omega_q + \frac{1}{4\pi}\int_{K_\rho} A(p,q)\left((c(q)+\lambda)u(q) - f(q)\right) d\omega_q$$

Let us now write (7) in the form

$$u(p) = \int_{K_\rho}\left[B_{0,0}(p,q) + B_{0,1}(p,q)\,\lambda\right] u(q)\,d\omega_q + d(p)$$

where $B_{0,0}(p,q) = \frac{1}{2\pi\rho^2}\cdot\frac{1}{r_{p,q}} + \frac{1}{4\pi}A(p,q)\,c(q)$

$B_{0,1}(p,q) = \frac{1}{4\pi}A(p,q)$

$d(p) = -\frac{1}{4\pi}\int_{K_\rho} A(p,q)f(q)\,d\omega_q = P_{1,\rho}(f)$

On iterating three times we obtain an equation of the form

$$(8)\quad u(p) = \sum_{\mu=0}^{4}\lambda^\mu \int_{K_\rho} B_\mu(p,q)\,u(q)\,d\omega_q + P(f)$$

where $P(f) = d_3(p)$

and where $P(f)$ is a functional linear and homogeneous in f independent of u and where the B_μ's are functions L_2 with respect to q if c(p) is L_2 in each finite domain.

III. CLASSIFICATION OF TYPES

Let us suppose that the second member of (1) is a function L_2 in the infinite space D_∞. Let us consider a set of spheres D_m having the origin as center and whose rays R_m tend toward infinity. If λ is non-real and if the coefficient of c(p) satisfies certain conditions of regularity large enough (which are verified if $\int|c(p)|^2 d\omega_p$ converges in each finite domain) it is known that (1) admits one and only one continuous solution $u_m(p)$ in D_m and satisfying on S_m (limiting surface of D_m) a condition on the limits of the form

$$(9)\quad \frac{\partial u}{\partial n} + a_m(p)\,u(p) + \int_{S_m} H_m(p,q)\,u(q)\,d\sigma_q = 0$$

where $a_m(p)$ is a real and continuous function and $H_m(p,q)$ is a continuous hermitian kernel.

Let us apply Green's formula (5) to u_m and $\bar{u}_m$. We have

$$(10)\quad \int_D \left[u_m L(\bar{u}_m) - \bar{u}_m L(u_m)\right] d\omega + \int_S \left[u_m\frac{\partial\bar{u}_m}{\partial n} - \bar{u}_m\frac{\partial u_m}{\partial n}\right] d\sigma = 0$$

Using (1) we have $L(u_m) = f - \lambda u_m$ and $L(\bar{u}_m) = \bar{f} - \bar{\lambda}\bar{u}_m$.

Substituting these in (10) we have

$$(10a)\quad \int_{D_m}\left[u_m(\bar{f}-\bar{\lambda}\bar{u}_m) - \bar{u}_m(f-\lambda u_m)\right] d\omega + \int_{S_m}\left[u_m\frac{\partial\bar{u}_m}{\partial n} - \bar{u}_m\frac{\partial u_m}{\partial n}\right] d\sigma = 0$$

or

$$(10b)\quad \int_{D_m}\left[(u_m\bar{f} - \bar{u}_m f) + (\lambda-\bar{\lambda})|u_m|^2\right] d\omega + \int_{S_m}\left[u_m\frac{\partial\bar{u}_m}{\partial n} - \bar{u}_m\frac{\partial u_m}{\partial n}\right] d\sigma = 0$$

Let us take (9) and multiply by $\bar{u}_{m_s}(p)$. We get

$$\bar{u}_m(p)\frac{\partial u_m}{\partial n} + a_m(p)|u_m(p)|^2 + \int_{S_m} H_m(p,q)\,u_m(q)\,\bar{u}_m(p)\,d\sigma_q = 0$$

Then we take the conjugate and obtain

$$u_m(p)\frac{\partial \bar{u}_m}{\partial n} + a_m(p)|u_m(p)|^2 + \int_{S_m} H_m(p,q)\,\bar{u}_m(q)\,u_m(p)\,d\sigma_q = 0$$

Let us subtract these last two equations and integrate with respect to p. We have

$$\int_{S_m}\left(\bar{u}_m(p)\frac{\partial u_m(p)}{\partial n} - u_m(p)\frac{\partial \bar{u}_m(p)}{\partial n}\right)d\sigma +$$

$$(11)\quad + \iint_{S_m S_m}\left[H_m(p,q)\,u_m(q)\,\bar{u}_m(p) - H_m(q,p)\,\bar{u}_m(q)\,u_m(p)\right]d\sigma_q\,d\sigma_p = 0$$

With attention to the double integral we find that

$$H_m(p,q)\,u_m(q)\,\bar{u}_m(p) - H_m(q,p)\,\bar{u}_m(q)\,u_m(p) = 0$$

Substituting this in (11) we obtain

$$\int_{S_m}\left(u_m(p)\frac{\partial \bar{u}_m(p)}{\partial n} - \bar{u}_m(p)\frac{\partial u_m(p)}{\partial n}\right)d\sigma_p = 0$$

Now substituting this in (10b) we obtain

$$(12)\quad (\lambda-\bar{\lambda})\int_{D_m}|u_m|^2\,dw = \int_{D_m}\bar{u}_m f\,dw - \int_{D_m} u_m \bar{f}\,dw$$

Taking absolute values and applying the inequality of Schwartz we obtain

$$(13)\quad \int_{D_m}|u_m|^2 dw \le \left|\frac{2}{\lambda-\bar{\lambda}}\right|^2 \int_{D_m}|f|^2 dw$$

u_m satisfying equations (7) and (8). By a theorem of Riesz (13) implies that $u_{m_s} \to u$ weakly and $\int |u|^2 dw \le A$. Referring to a theorem of Riesz in regard to passing to the limit under the integral sign and noticing that our integral equation (8) is of the same form and same conditions are fulfilled as the function in the theorem of Riesz we can assert that $u_m(p)$ converges in the ordinary sense in K_ρ and over the whole space. There exists at least one solution L_2 of (1) for λ non-real.

There follows now a classification of the differential expressions $L(u)$. $L(u)$ is said to be of the determinate type or indeterminate type according as the equation $L(u) + \lambda u = 0$ does not admit or admit a solution non-null and L_2 for λ non-real. We have the following theorem:

Let E be the set of functions $u \subset L_2$ such that $L(u)$ be also L_2. This puts the necessary and sufficient condition for $L(u)$ to be of determinate type that we have

(14) $\int_{\Omega} v\,L(u)\,d\omega = \int_{\Omega} u\,L(v)\,d\omega$

each time that u and v are in E.

1. The condition is sufficient. If the theorem fails, we have a function u so that

(1a) $\lambda u + L(u) = 0$ and $\int_{\Omega} |u|^2 d\omega \neq 0$

where $\lambda = \alpha + i\beta$, $\beta \neq 0$

By (1a)

(1b) $\bar{\lambda}\bar{u} + L(\bar{u}) = 0$

Let us multiply (1a) by $\bar{u}$ and (1b) by u. We have

$\lambda |u|^2 + \bar{u}\,L(u) = 0$

(1c) $\bar{\lambda} |u|^2 + u\,L(\bar{u}) = 0$

We integrate (1c)

$\lambda \int |u|^2 d\omega + \int \bar{u}\,L(u)\,d\omega = 0$

$\bar{\lambda} \int |u|^2 d\omega + \int u\,L(\bar{u})\,d\omega = 0$

We subtract these and obtain

$(\lambda - \bar{\lambda}) \int |u|^2 d\omega = 0$

and a contradiction if

(1d) $\int \bar{u}\,L(u)\,d\omega = \int u\,L(\bar{u})\,d\omega$

for all $u \subset L_2$ such that $L(u) \subset L_2$. (i.e. for all $u \subset E$; if $u \subset E$ then $\bar{u} \subset E$)

But (1d) holds by hypothesis.

2. The condition is necessary. We must show that

$$\int_{\Omega} u\,L(v)\,d\omega = \int_{\Omega} v\,L(u)\,d\omega$$

if $L(u)$ is of determinate type and if $u, v, L(u), L(v) \subset L_2$

Let λ^* be a non-real quantity. We define the functions $f_1(x)$ and $f_2(x)$ as follows

$f_1(x) = L(u) + \lambda^* u \quad \subset L_2$

(2a) $f_2(x) = L(v) + \lambda^* v \quad \subset L_2$

It follows from a theorem concerning use of transformation of such functions that

(2b) $\int_{\Omega} u\,f_2(x)\,d\omega = \int_{\Omega} v\,f_1(x)\,d\omega$

where $u = T(f_1)$, $v = T(f_2)$

Since equation is of the determinate type - then

substituting for $f_2(x)$ and $f_1(x)$ we have

$$(2c)\quad \int_{\Omega_0} (u\,L(v) + \lambda^* uv)\,d\omega = \int_{\Omega_0} (v\,L(u) + \lambda^* vu)\,d\omega$$

whence

$$\int_{\Omega_0} u\,L(v)\,d\omega = \int_{\Omega_0} v\,L(u)\,d\omega.$$

IV. DETERMINATE TYPE

Let us suppose now that $L(u)$ is of the determinate type and return to the problem of the limits (9) relative to the domain Ω_m. According to the classical theory we know that the equation

$$L(u) + \lambda u = 0$$

with condition (9) admits no solutions non-null continuous that satisfy the condition (9) except for a set of real values λ_j not having a limit point of finite distance. The corresponding fundamental functions $\varphi_j^{(m)}(p)$ can be normalized in a manner such that they form a complete ortho-normal system.

Let us introduce the spectral function $\theta_m(p, q \mid \lambda)$ defined by the following relations:

$$\theta_m(p, q \mid \lambda) = \sum_{0 \le \lambda_j \le \lambda} \varphi_j^{(m)}(p)\,\varphi_j^{(m)}(q) \quad , \lambda > 0$$

(15)

$$\theta_m(p, q \mid \lambda) = \sum_{\lambda \le \lambda_j < 0} \varphi_j^{(m)}(p)\,\varphi_j^{(m)}(q) \quad , \lambda \le 0$$

On applying (8) we find

$$(16)\quad \varphi_j^{(m)}(p) = \sum_{\mu=0}^{4} \lambda_j^{\mu} \int_{K_{p'}} B_\mu(p, p_1)\,\varphi_j^{(m)}(p_1)\,d\omega_{p_1}$$

On putting $\Delta\theta_m(p, q \mid \lambda) = \theta_m(p, q \mid \lambda + \Delta\lambda) - \theta_m(p, q \mid \lambda)$ it follows that

$$(17)\quad \Delta\theta_m(p, q \mid \lambda) = \sum_{\mu_1=0}^{4} \sum_{\mu_2=0}^{4} \int_{\Delta} \lambda^{\mu_1+\mu_2} d_\lambda \iint_{K_{p'}\,K_{q'}} \theta_m(p_1, q_1 \mid \lambda) \cdot$$

$$\cdot B_{\mu_1}(p, p_1)\,B_{\mu_2}(q, q_1)\,d\omega_{p_1}\,d\omega_{q_1}.$$

With this expression or relation and the following inequality

$$0 \leq \iint_{D_m D_m} \Delta\,\theta_m(p,q\,|\,\lambda)\,h(p)\,h(q)\,d\omega_p\,d\omega_q \leq \int_{D_m} h(p)^2\,d\omega_p$$

given by Carleman in his book (C) the fact is deduced that $\theta_m(p,q\,|\,\lambda)$ is a function of bounded variation in each finite interval and that its variation is less than a constant independent of m and that we can choose a set of integers m_ν such that

$$\lim_{m_\nu \to \infty} \theta_m(p,q\,|\,\lambda) = \theta(p,q\,|\,\lambda) \quad \text{exists.}$$

In the determinate case the limit $\theta(p,q\,|\,\lambda)$ is the same whatever be the set m_ν and whatever be the functions a_m and H_m in (9). Let $v < E$ be a real function L_2 in D_∞ such that $L(v) = f$ be also L_2. One can choose the functions a_m and H_m in (9) in such a manner that v satisfies (9). We express the Fourier expansion of v in D_m in terms of the complete ortho-normal set $\varphi_\nu^{(m)}$ for all v and p in D_m. We have

$$(18)\quad v(p) = \int_{-\infty}^{\infty} d_\lambda \int_{D_m} \theta_m(p,q\,|\,\lambda)\,v(q)\,d\omega_q = -\int_{-\infty}^{\infty} \frac{1}{\lambda}\,d_\lambda \int_{D_m} \theta_m(p,q\,|\,\lambda)\,f(q)\,d\omega_q$$

By the use of the spectral functions and formula (14) we show the second equality. We can also write

$$(19)\quad v(p) = \int_{-\infty}^{\infty} d_\lambda \int_{D_\infty} \theta(p,q\,|\,\lambda)\,v(q)\,d\omega_q = -\int_{-\infty}^{\infty} \frac{1}{\lambda}\,d_\lambda \int_{D_\infty} \theta(p,q\,|\,\lambda)\,f(q)\,d\omega_q$$

which is the generalized Fourier expansion of arbitrary v.

In (C) Carleman announces that in the determinate case there exists one and essentially only one spectral function $\theta(p,q\,|\,\lambda)$ continuous and L_2 with respect to p and with respect to q and of bounded variation with respect to λ such that we have

$$(20)\quad \int_{-\infty}^{\infty} d_\lambda \iint_{D_\infty D_\infty} \theta(p,q\,|\,\lambda)\,h(p)\,h(q)\,d\omega_p\,d\omega_q = \int_{D_\infty} h(p)^2\,d\omega_p$$

$$(21)\quad \int_{-\infty}^{\infty} h(\lambda)^2\,d_\lambda \iint_{D_\infty D_\infty} \theta(p,q\,|\,\lambda)\,h(p)\,h(q)\,d\omega_p\,d\omega_q =$$

$$= \int_{D_\infty} \left[\int_{-\infty}^{\infty} d_\lambda \int_{D_\infty} \theta(p,q\,|\,\lambda)\,h(q)\,d\omega_q \right]^2 d\omega_p.$$

If v is any function whatever L_2 we have

$$(22)\quad v(p) \sim \int_{-\infty}^{\infty} d_\lambda \int_{D_\infty} \theta(p,q\,|\,\lambda)\,v(q)\,d\omega_q$$

The sign $\sim$ indicates that the integral $\int_{-\infty}^{\infty}$ of the second member converges in the mean to $v(p)$.

We show that (22) follows from (20) by use of Parseval's relation and the Riesz-Fischer theorem.

If $L(v)=f$ is L_2 and v is L_2 in like manner using (21) we have the following relation:

$$(23)\quad L(v) \sim \int_{-\infty}^{\infty} \lambda \, d_\lambda \int_{D_\lambda} \Theta(p,q\,|\lambda)\, v(q)\, d\omega_q .$$

VITA

David Wright Starr was born in Anna, Texas, December 8, 1912. He was graduated from Denison High School, Denison, Texas, in 1929. From 1929-33 he attended Southern Methodist University and received the degree of Bachelor of Arts there in 1933. The year 1933-34 he was a teacher at Sadler High School, Sadler, Texas, and was principal there at the beginning of the next school year. He went to Denison High School in 1934 and served as teacher of mathematics there during the years 1934-37. He attended the University of Illinois the summers of 1934-35-36-37 and received the degree of Master of Arts there in August, 1937. At the University of Illinois during the year 1937-38 he held a fellowship and during the years 1938-40 he was an assistant in mathematics.